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A Compact Analytical Fit to the Exponential Integral $E_1(x)$

by Steven B. Segletes

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A Compact Analytical Fit to the Exponential Integral $E_1(x)$

Steven B. Segletes

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Abstract

A four-parameter fit is developed for the class of integrals known as the exponential integral (real branch). Unlike other fits that are piecewise in nature, the current fit to the exponential integral is valid over the complete domain of the function (compact) and is everywhere accurate to within $\pm 0.0052\%$ when evaluating the first exponential integral, E_1 . To achieve this result, a methodology that makes use of analytically known limiting behaviors at either extreme of the domain is employed. Because the fit accurately captures limiting behaviors of the E_1 function, more accuracy is retained when the fit is used as part of the scheme to evaluate higher-order exponential integrals, E_n , as compared with the use of brute-force fits to E_1 , which fail to accurately model limiting behaviors. Furthermore, because the fit is compact, no special accommodations are required (as in the case of spliced piecewise fits) to smooth the value, slope, and higher derivatives in the transition region between two piecewise domains. The general methodology employed to develop this fit is outlined, since it may be used for other problems as well.

Acknowledgments

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1. Introduction

A number of useful integrals exist for which no exact solutions have been found. In other cases, an exact solution, if found, may be impractical to utilize over the complete domain of the function because of precision limitations associated with what usually ends up as a series solution to the challenging integral. For many of these integrals, tabulated values may be published in various mathematical handbooks and articles. In some handbooks, fits (usually piecewise) also are offered. In some cases, an application may be forced to resort to numerical integration in order to acquire the integrated function. In this context, compact (*i.e.*, not piecewise) analytical fits to some of these problematic integrals, accurate to within a small fraction of the numerically integrated value, serve as a useful tool to applications requiring the results of the integration, especially when the integration is required numerous times throughout the course of the application. Furthermore, the ability and methodology to develop intelligent fits, in contrast to the more traditional “brute force” fits, provide the means to minimize parameters and maximize accuracy when tackling some of these difficult functions. The exponential integral will be used as an opportunity to both demonstrate a methodology for intelligent fitting as well as for providing an accurate, compact, analytical fit to the exponential integral.

The exponential integral is a useful class of functions that arise in a variety of applications, including the theory of interatomic energy potentials [1], the theory of lethal areas for fragmenting warheads [2], and the theory of ballistic penetration [3], to name but a few. The real branch of the family of exponential integrals may be defined by

$$E_n(x) = x^{n-1} \int_x^{\infty} \frac{e^{-t}}{t^n} dt , \quad (1)$$

where n , a positive integer, denotes the specific member of the exponential-integral family. The argument of the exponential integral, rather than expressing a lower limit of integration as in

eqn(1), may be thought of as describing the exponential decay constant, as given in this equivalent (and perhaps more popular) definition of the integral:

$$E_n(x) = \int_1^{\infty} \frac{e^{-xt}}{t^n} dt \quad (2)$$

Integration by parts permits any member of the exponential-integral family to be converted to an adjacent member of the family, by way of

$$\int_x^{\infty} \frac{e^{-t}}{t^{n+1}} dt = \frac{1}{n} \left(\frac{e^{-x}}{x^n} - \int_x^{\infty} \frac{e^{-t}}{t^n} dt \right), \quad (3)$$

expressable in terms of E_n as

$$E_{n+1}(x) = \frac{1}{n} \left[e^{-x} - x E_n(x) \right] \quad (n=1, 2, 3...) \quad (4)$$

Through recursive employment of eqn (4), all the members of the exponential integral family may be analytically related. However, this technique only allows for the transformation of one integral into another. There remains the problem of evaluating $E_1(x)$. There is an exact solution to the integral of (e^{-t}/t) , appearing in a number of mathematical references [4, 5], which is obtainable by expanding the exponential into a power series and integrating term by term. That exact solution, which is convergent, may be used to specify $E_1(x)$ as

$$E_1(x) = -\gamma - \ln(x) + \frac{x}{1!} - \frac{x^2}{2 \cdot 2!} + \frac{x^3}{3 \cdot 3!} - \dots \quad (5)$$

Euler's constant, γ , equal to 0.57721..., arises in eqn (5) when the power-series expansion for (e^{-t}/t) is integrated and evaluated at its upper limit, as $x \rightarrow \infty$ [6].

Employing eqn (5), however, to evaluate $E_1(x)$ is problematic for finite x significantly larger than unity. One might well ask of the need to evaluate the exponential integral for large x , since the function to be integrated drops off so rapidly that the integral is surely a very flat function. Such reasoning is true when comparing the integrand at large x to that at small x . However, the definition of eqn (1) has as its upper limit not a small value of x , but rather that of ∞ . Therefore, the actual values for $E_n(x)$ are extremely small numbers for large values of x . Thus, it is not sufficient merely to select enough terms of eqn (5) to evaluate the integral to within a value of, for example, ± 0.0001 because the actual integral value for large x would be smaller than this arbitrary tolerance. To draw an analogy, it would be like saying that it is good enough to approximate e^{-x} as 0.0 for $x > 10$, since its actual value is within 0.0001 of zero. For some applications, such an approximation may be warranted. In general, though, such an approximation is mathematically unacceptable. Worse yet, as seen from eqns (1) and (2), the need to evaluate the exponential integral for large arguments can arise in real-world problems from either a large integration limit or a large value of an exponential decay constant. Thus, the need to evaluate exponential integrals for large values of the argument is established. It is here that the practical problems with the evaluation of eqn (5) become manifest.

First, the number of terms, N , required to achieve convergence rises rapidly with increasing x , making the summation an inefficient tool, even when expressed as a recursion relation (for three digits of accuracy, N is observed to vary roughly as $9 + 1.6x$, for $1 < x < 7$). More important, however, is the fact that, for calculations of finite precision, the accuracy of the complete summation will be governed by the individual term of greatest magnitude. The source of the problem is that as x is increased, the total summation decreases in magnitude more rapidly than a decaying exponential, while at the same time, the largest individual term in the series is observed to grow rapidly with increasing x ($\sim 10^1$ for $x = 7$, $\sim 10^2$ for $x = 10$, $\sim 10^3$ for $x = 13$, *etc.*). The magnitude of this largest individual term consumes the available precision and, as a result, leaves little or none left for the ever-diminishing net sum that constitutes the desired integral.

Literally, the use of eqn (5), even with (32-bit) double precision, does not permit the exponential integral to be evaluated to three places for $x > 14$ in any case, and with the situation worsening for lesser precision. For these reasons, the use of eqn (5) to evaluate the exponential integral numerically for large x is wholly unsuitable.

Others have obviously recognized this problem, as the exponential integral in some handbooks [5] receives a whole chapter of attention. For large x , a continued fraction exists that converges to the integral, given by

$$E_1(x) = e^{-x} \cdot \frac{1}{x + \frac{1}{1 + \frac{1}{x + \frac{2}{1 + \frac{2}{x + \dots}}}}} \quad (6)$$

But as x becomes smaller, the number of terms required for convergence rises quickly. Similar arguments apply for the use of an asymptotic expansion for E_1 , which also converges for large x . As such, the more typical approach employed by handbooks is that of a fit. While some steps are taken to make the fits intelligent (*e.g.*, transformation of variables), the fits are all piecewise over the domain of the integral.

Cody and Thatcher [7] have performed what is perhaps the definitive work, with the use of Chebyshev approximations to the exponential integral E_1 . Like others, they fit the integral over a piecewise series of subdomains (three in their case) and provide the fitting parameters necessary to evaluate the function to various required precisions, down to relative errors of 10^{-20} . One of the problems with piecewise fitting over two or more subdomains is that functional value and derivatives of the spliced fits will not, in general, match at the domain transition point, unless special accommodations are made. This sort of discontinuity in functional value and/or slope, curvature, *etc.*, may cause difficulties for some numerical algorithms operating upon the fitted function. Numerical splicing/smoothing algorithms aimed at eliminating discontinuities in the

value and/or derivatives of a piecewise fit are not, in general, computationally insignificant. Problems associated with piecewise splicing of fits may also be obviated by obtaining an accurate enough fit, such that the error is on the order of magnitude of the limiting machine precision. This alternative, however, requires the use of additional fitting parameters to acquire the improved precision. Thus, regardless of approach, the desire to eliminate discontinuities in the function and its derivatives, between piecewise splices, requires extra computational effort. One final benefit to be had by avoiding the use of piecewise fits is the concomitant avoidance of conditional (*i.e.*, IF...THEN) programming statements in the coding of the routine. The use of conditional statements can preclude maximum computing efficiency on certain parallel computing architectures.

Therefore, an alternate method is devised to approximate the exponential integral. A compact, analytical fit that strives to predict the exponential integral to within a small percentage of the actual value is sought. Ideally, the fit will remain accurate over all x , which will distinguish it from other, piecewise, fits to the exponential integral.

2. The Approach

Since large values of x ($x > 1$) are the root of the current difficulty, this paper first focuses on that region of the domain. Fitting any function accurately over the expansive domain $x > 1$ can be a daunting task. Even more so is the family of exponential integrals, eqn (1), which experience drastic order of magnitude changes over that domain. To map the infinite into an acceptably small, finite domain, transform the exponential integrals by way of the substitution $w = 1/x$ (and transform the dummy variable, t , by way of $u = 1/t$). In this manner, the domain $x > 1$ maps into the transformed domain $0 < w < 1$, which is much more amenable to study. (Of course, the downside is that values of $x < 1$ transform into the expansive domain $w > 1$.) With this simple substitution, the family of exponential integrals given by eqn (1) becomes

$$E_n(w = 1/x) = \frac{1}{w^{n-1}} \int_0^w u^{n-2} e^{-1/u} du \quad . \quad (7)$$

Eqn (7) is then numerically integrated with respect to u for several representative values for n (using Simpson's Rule, with a step size of 1×10^{-7} across the small- w domain), so as to obtain a better understanding of the function. At small w (less than 0.0016, corresponding to $x = 625$), the ability of double precision (64 computer bits) to represent the tiny exponentials is at its limit. For the three logarithmic cycles of w between 0.001 and 1, the exponential integral E_1 varies by more than 300 orders of magnitude. Figure 1 shows several of these integrals over 40 of those orders of magnitude. Clearly, a transformation is required to collapse this vast change in scale into something less dramatic. Such a transformation is found, when it is realized that

$$\lim_{w \rightarrow 0} \frac{E_n}{w e^{-1/w}} = 1 \quad . \quad (8)$$

Therefore, E_n is transformed by way of the relation $F_n = E_n / (w e^{-1/w})$. In this way, F_n equals unity, when evaluated at $w = 0$. Figure 2 depicts F_1 , F_2 , and F_3 over several subdomains of w . It is observed from Figure 2a that, even though the values of E_n cannot be evaluated using double-precision arithmetic for w much below $w = 0.0016$, the transformation of E_n into F_n allows for an excellent interpolation between the (w, F_n) point (0,1) and small values of w since, unlike E_n , the behavior of F_n at low w is nearly linear. As observed from Figure 2a, the initial slopes of F_1 , F_2 , and F_3 appear to be -1 , -2 , and -3 , respectively. To obtain these values exactly, let $F_n = 1 - a_n w + b_n w^2 - \dots$ for infinitesimal w . Substituting the definition for F_n (and with the use of eqn [7]) results in

$$w^{n-1} E_n = \int_0^w u^{n-2} e^{-1/u} du = w^n e^{-1/w} (1 - a_n w + b_n w^2 - \dots) \quad . \quad (9)$$

By taking the derivative of this expression and collecting terms, a_n must equal n , and b_n must equal $n(n+1)$ in the small- w limit. These derived values for a_n confirm the slope observations from Figure 2a.

Rather than attempting a fit to the F_n directly, however, the quantity $F_1 \cdot w$ is first plotted in Figure 3. At large w , the curve appears to be logarithmic in nature, in comparison to the curve

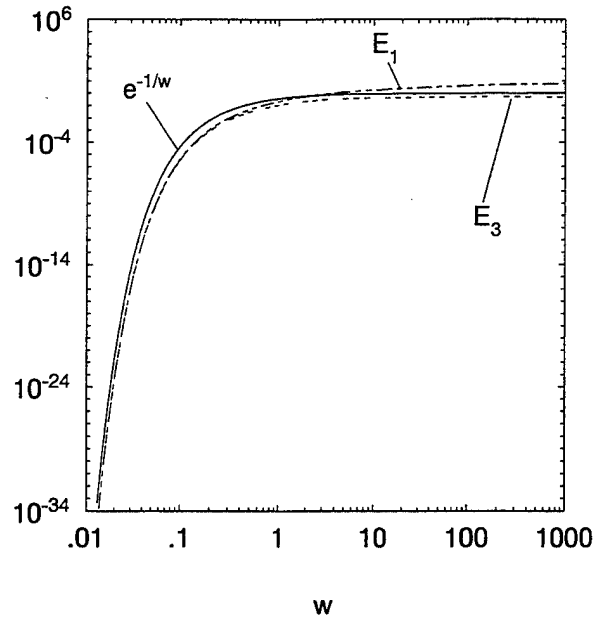
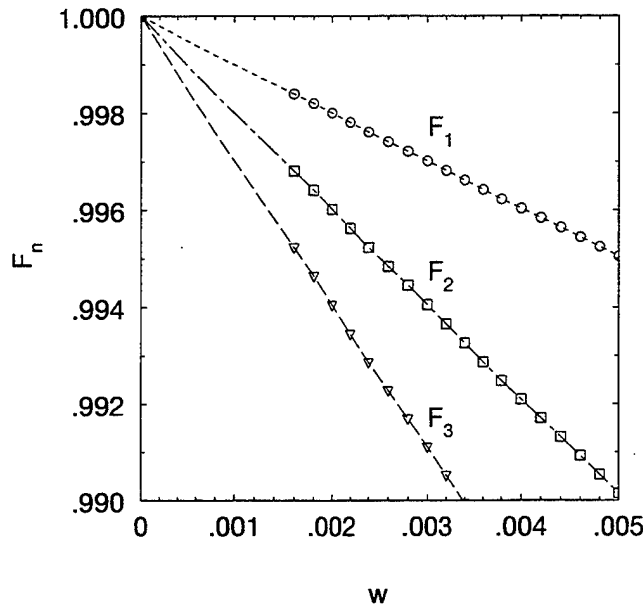
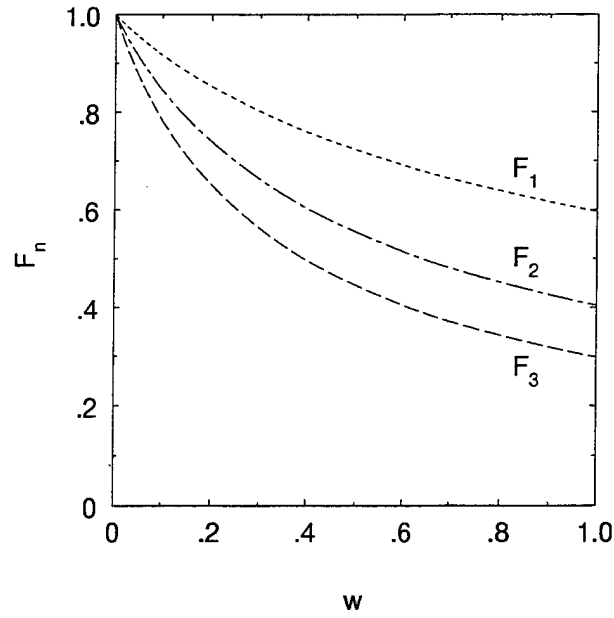


Figure 1. The exponential integrals E_1 and E_3 expressed in terms of $w = 1/x$, in relation to the decaying exponential function.

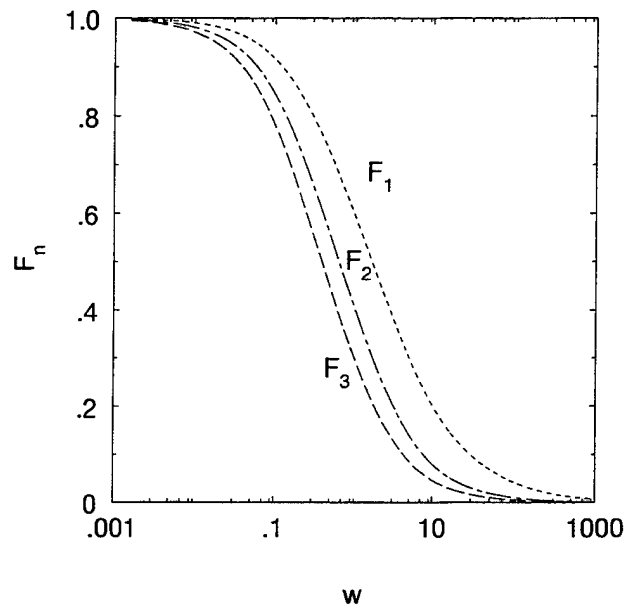


(a)

Figure 2. The functions F_1 , F_2 , and F_3 , (a) in the small- w limit, corresponding to $x \rightarrow \infty$; (b) over the domain $0 < w < 1$, corresponding to $x > 1$; (c) over six logarithmic cycles of w , corresponding to $0.001 < x < 1000$.



(b)



(c)

Figure 2. The functions F_1 , F_2 , and F_3 , (a) in the small- w limit, corresponding to $x \rightarrow \infty$; (b) over the domain $0 < w < 1$, corresponding to $x > 1$; (c) over six logarithmic cycles of w , corresponding to $0.001 < x < 1000$.

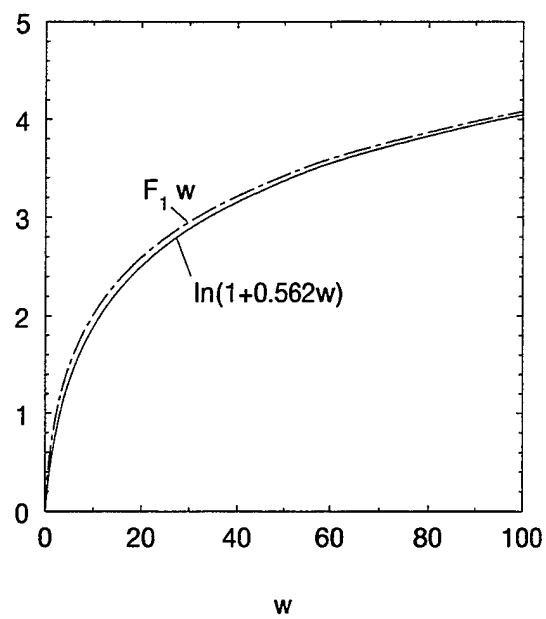


Figure 3. A comparison of $F_1 \cdot w$ to $\ln(1+0.562w)$, for larger w , above unity.

$\ln(1 + 0.562 w)$, shown in the same figure. Large values of w correspond to small x , where eqn (5) is more easily evaluated. From the nature of eqn (5) as x approaches zero, it is seen that

$$\lim_{x \rightarrow 0} E_1(x) = -\gamma - \ln(x) \quad (10)$$

From eqn (10), by transforming x to $1/w$ and E_1 to $(F_1 \cdot w)/e^{-1/w}$, a comparison of the term $F_1 \cdot w$ to the functional form $\ln(1+kw)$, as $w \rightarrow \infty$, reveals that k must take on the exact value $e^{-\gamma} = 0.5615...$

However, for small w , the form $\ln(1+e^{-\gamma} w)$ is not appropriate. Rather, recall that, for small w , the functions F_n are shown to be of the limiting form $1 - n w + n(n+1)w^2$. Thus, for the case of $n = 1$ (the lowest-order exponential integral), $F_1 \cdot w$ must follow as $w - w^2 + 2w^3$ for small w . A Taylor-series expansion of $\ln(1+e^{-\gamma} w)$ about $w = 0$, by contrast, is given (to two terms) by the form $e^{-\gamma} w - 1/2 \cdot e^{-2\gamma} w^2$. As compared to $w - w^2 + 2w^3$, the Taylor expansion is observed to have the wrong initial slope ($e^{-\gamma}$, instead of 1.0) and curvature ($-e^{-2\gamma}$, as compared with the proper value of -2) in the low- w limit. To remedy the slope and curvature mismatch, compare in Figure 4 the function $F_1 \cdot w$ to a different logarithmic form (one possessing the proper initial slope of 1 and curvature of -2)—namely, the function $\ln[1+\ln(1+w)]$, which provides an excellent low- w approximation to $F_1 \cdot w$ by matching the value, slope, and curvature of $F_1 \cdot w$.

Therefore, the limiting behavior of $F_1 \cdot w$ is known for both $w \rightarrow 0$ as well as $w \rightarrow \infty$. As such, the fitting strategy for $F_1 \cdot w$ is now apparent: a form which follows $\ln[1+\ln(1+w)]$ for low w and transitions to $\ln(1+e^{-\gamma} w)$ for larger w . There are a number of ways in which this transition might be accomplished, but, after some study, the following explicit form that exhibits the sought-after characteristics has been chosen:

$$F_1 \cdot w \approx \ln\{1 + w - [w - \ln(1 + w)] \cdot f(w)\} \quad (11)$$

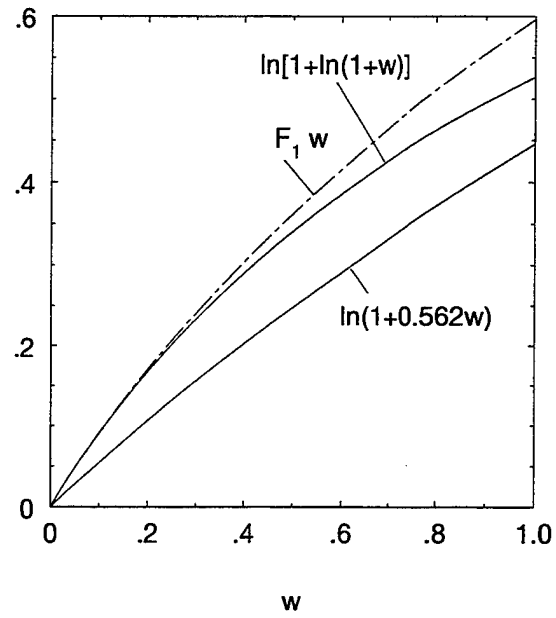


Figure 4. A comparison of $F_1 \cdot w$ to $\ln[1+\ln(1+w)]$ and $\ln(1+0.562w)$, for small w , below unity.

where $f(w)$ is the function to parameterize and fit. One alternative strategy, that of having two fitting functions (f_1 to transition down the low- w form and f_2 to activate the large- w solution), is discarded for two reasons: (1) more fitting parameters are required for two transition functions, as compared to one; and (2) $f_1 \cdot \ln(1+w)$ and $f_2 \cdot e^{-\gamma} w$ interact in a nonlinear way, making it difficult to avoid excessive slope and curvature oscillations in the transition region. By contrast, the form selected in eqn(11) has three primary virtues above many other fitting forms: (1) it requires only a single function to be fit, thereby minimizing the number of fitting parameters; (2) as w increases, the logarithmic term in brackets naturally exhibits diminished importance with respect to the linear term, thereby providing an automatically smooth transition to the high- w solution; and (3) because at small w the logarithmic term behaves like w and monotonically diverges from it thereafter, the value and *every* higher derivative of the quantity $[w - \ln(1+w)]$ exhibit smooth, monotonic behavior. Such monotonicity helps to ensure that the behavior of f is also smooth and monotonic.

Recalling that $F_1 \cdot w$ is identical to $E_1/e^{-1/w}$, the first three exponential integrals may be given, in terms of $f(w)$, as

$$E_1 = \int_0^w \frac{e^{-1/u}}{u} du \approx e^{-1/w} \cdot \ln \{ 1 + w - [w - \ln(1+w)] \cdot f(w) \} , \quad (12a)$$

$$E_2 = \frac{1}{w} \int_0^w e^{-1/u} du \approx \frac{e^{-1/w}}{w} (w - \ln \{ 1 + w - [w - \ln(1+w)] \cdot f(w) \}) , \quad (12b)$$

and

$$E_3 = \frac{1}{w^2} \int_0^w u e^{-1/u} du \approx \frac{e^{-1/w}}{2 w^2} (w^2 - w + \ln \{ 1 + w - [w - \ln(1+w)] \cdot f(w) \}) . \quad (12c)$$

Higher-order exponential integrals may be determined, after a similar fashion, with the use of eqn (4), expressed in w .

3. The Fit(s)

From eqn (11), $f(0) = 1$, in order to have the proper low- w behavior. At larger w , f should approach the constant value of $(1 - e^{-\gamma}) = 0.4385...$ Furthermore, recall that for infinitesimal w , $F_1 \cdot w$ follows the form $w - w^2 + 2w^3$. And though the low- w stencil, $\ln[1 + \ln(1 + w)]$, matches the limiting value, slope, and curvature of $F_1 \cdot w$, the initial slope of f may be further restricted to force a match to the third derivative of $F_1 \cdot w$, as well. By equating this limiting cubic form to the right side of eqn (11), the third derivative may be taken (tedious though it may be) to show that $12 = -3f_0' + 7$, or

$$f_0' = -5/3 \quad . \quad (13)$$

The numerically integrated values for E_1 are used to generate explicit values for f , as shown in Figure 5. To achieve a fit to this data, an appropriate functional form is needed to approximate the explicit data shown in Figure 5. Two forms are now presented. The simplest, with two free parameters, is

$$f(w) = \frac{(1 + Aw + (1 - e^{-\gamma})Bw^2)}{(1 + (A + 5/3)w + Bw^2)} \quad . \quad (14)$$

This function begins at unity, for $w = 0$, has an initial slope of $-5/3$, and asymptotes to $(1 - e^{-\gamma})$ for large w , thus satisfying both the small- and large- w asymptotic requirements. The value of B relative to A helps to determine the magnitude of the transition region.

The quality of this fit may be compared to the numerically integrated values and be expressed as a maximum percent-deviation from the integrated value, as in

$$\% \text{ Error} = 100 \times \max[(E_n)_{fit} - E_n] / E_n \quad . \quad (15)$$

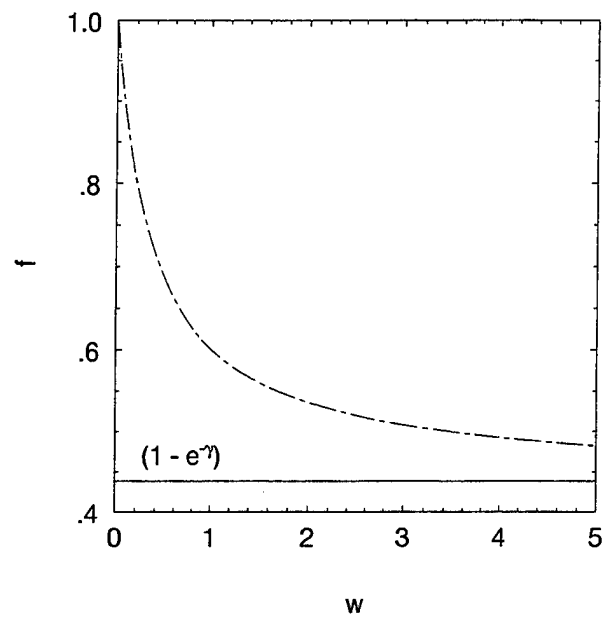


Figure 5. A graph of the f function to be fit, showing a limiting value of unity as $w \rightarrow 0$, and the asymptote, $f = (1 - e^{-\gamma})$, corresponding to large w .

Over the complete domain of the function, the resulting fit (attempting to minimize the percent error in E_1) to this two-parameter version of f is given as

$$f(w) = \frac{1 + 5.874w + (1 - e^{-\gamma}) \cdot 10.8w^2}{1 + (5.874 + 5/3)w + 10.8w^2}, \quad 0 < w < \infty \quad (E_1 \text{ within } \pm 0.067\%). \quad (16a)$$

Restricting the fit to the subdomain $0 < w < 1$ ($x > 1$), as do many of the existing fits, results in

$$f(w) = \frac{1 + 4.311w + (1 - e^{-\gamma}) \cdot 6.851w^2}{1 + (4.311 + 5/3)w + 6.851w^2}, \quad 0 < w < 1 \quad (E_1 \text{ within } \pm 0.002\%). \quad (16b)$$

A four-parameter form is also developed for f , given by

$$f(w) = \frac{1 + 4.054w + (1 - e^{-\gamma}) \cdot 6.207w^2}{1 + (4.054 + 5/3)w + [1 + 0.5032w/(29.3 + w)^2] \cdot 6.207w^2}, \quad 0 < w < \infty$$

(E_1 within $\pm 0.00511\%$). (16c)

Expressing eqn (12a) in terms of x , E_1 may be given as

$$E_1(x) = \int_x^\infty \frac{e^{-t}}{t} dt \approx e^{-x} \cdot \ln \{ 1 + 1/x - [1/x - \ln(1 + 1/x)] \cdot f(x) \}, \quad (17)$$

with $f(x)$ given as

$$f(x) = \frac{x^2 + 5.874x + (1 - e^{-\gamma}) \cdot 10.8}{x^2 + (5.874 + 5/3)x + 10.8}, \quad 0 < x < \infty \quad (E_1 \text{ within } \pm 0.067\%), \quad (18a)$$

$$f(x) = \frac{x^2 + 4.311x + (1 - e^{-\gamma}) \cdot 6.851}{x^2 + (4.311 + 5/3)x + 6.851}, \quad 1 < x < \infty \quad (E_1 \text{ within } \pm 0.002\%), \quad (18b)$$

or

$$f(x) = \frac{x^2 + 4.054x + (1 - e^{-\gamma}) \cdot 6.207}{x^2 + (4.054 + 5/3)x + [1 + 0.5032x/(1 + 29.3x)^2] \cdot 6.207}, \quad 0 < x < \infty$$

(18c)

Expressed in FORTRAN, this fit to E_1 may be coded in a single statement as

```

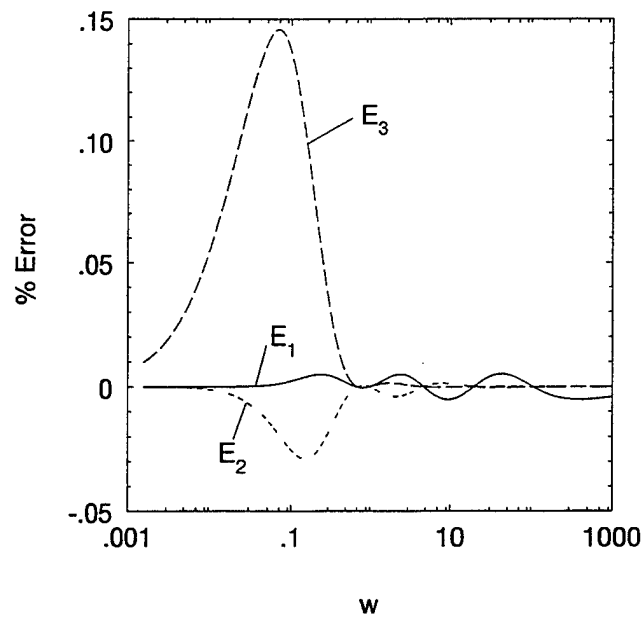
E1 = EXP(-X) * LOG(1. + 1./X - (1./X - LOG(1. + 1./X))
&      *(X**2 + 4.054*X + 2.72202)
&      /(X**2 + 5.72067*X + (1. + 0.5032*X/(1. + 29.3*X)**2)*6.207) )

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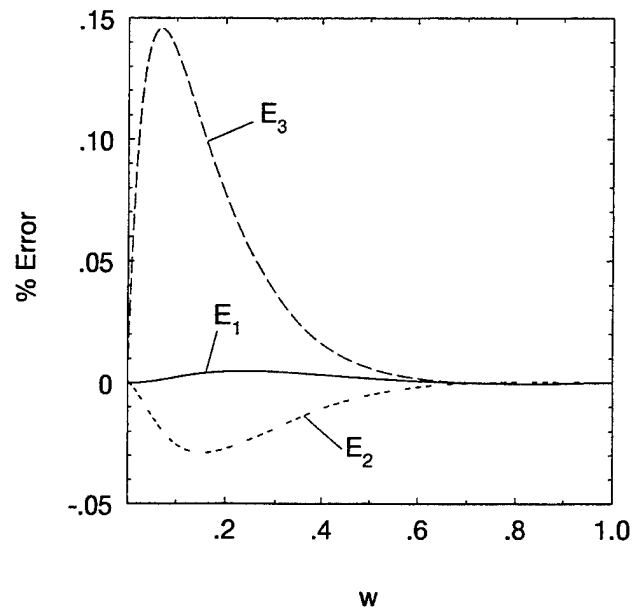
To reiterate, this fit is valid over the real domain of E_1 , $x > 0$, to within an error of $\pm 0.00511\%$. There is no need for conditional branching based on the value of x . Indeed, there is hardly a need to make the calculation external to the calling routine.

4. Quality of Fit

The accuracy for each of the fits to f is expressed in eqn (18) in terms of the maximum percent deviation of the fitted E_1 from its numerically integrated value. Because of the manner in which E_1 terms interact with higher-order exponential integrals [see eqn (4)], the error produced when using the fitted f to compute these higher-order integrals will differ from that of E_1 . Using the four-parameter eqn (18c) to conduct the comparison of E_1 , E_2 , and E_3 (i.e., eqns [12]) with the integrated data, Figure 6a reveals errors never exceeding $\pm 0.15\%$. Recall that any one of these exponential integrals varies by more than 300 orders of magnitude over the domain shown ($0.001 < w < 1000$) in Figure 6a. Figure 6b shows the same data (in linear scale) but focuses upon the domain $0 < w < 1$. Over this domain, corresponding to $x > 1$, the error is strictly less than $\pm 0.005\%$ for E_1 , $\pm 0.029\%$ for E_2 , and $\pm 0.15\%$ for E_3 .



(a)



(b)

Figure 6. The percent-error of the compact analytical fit, when used to evaluate E_1 , E_2 , and E_3 , (a) shown over six logarithmic cycles of w ; (b) over the domain $0 < w < 1$.

By contrast, a four-parameter fit to F_1 published by the (former) U.S. National Bureau of Standards (NBS) [5] (now the National Institute of Standards and Technology), given by

$$F_1 \approx \frac{x^2 + 2.334733x + 0.250621}{x^2 + 3.330657x + 1.681534}, \quad (19)$$

is valid only for the limited domain of $w < 1$ ($x > 1$) and has an absolute error band in F_1 of ± 0.00005 (expressed in terms of percent error in E_1 , it is $\pm 0.0051\%$). The four-parameter eqn (18c) betters this number with $\pm 0.005\%$, over the domain $x > 1$, as shown in Figure 7. Even the two-parameter eqn (18b), when restricted to the limited domain of $w < 1$ ($x > 1$), betters the NBS four-parameter fit by a factor of 2.5. To achieve a better accuracy than the current fit, the National Bureau of Standards specifies an eight-parameter fit in double precision which, again, is valid over only a limited subdomain of the function. At the other end of the functional domain (small x), compare the current four-parameter fit to eqn (5) when truncated to, for example, the cubic term. In this case, the current fit is more accurate for $x > 0.2$ ($w < 5$).

Furthermore, because the NBS fit fails to achieve the proper limiting derivatives as w approaches zero ($x \rightarrow \infty$), the use of the NBS fit to acquire the higher-order exponential integrals, by way of eqn (4) results in larger errors as $w \rightarrow 0$, whereas errors with the current fit approach zero as $w \rightarrow 0$. For example, E_2 has a limiting error in excess of -0.4% with the NBS fit (compared with a maximum error of $\pm 0.029\%$ with the current fit), and E_3 has a limiting error in excess of $+120\%$ (compared with a maximum error of $\pm 0.15\%$ for the current fit).

A comparison of the current fit to those published by Cody and Thatcher [7] is completely similar to that of the NBS, both in trend and in order of magnitude. To exceed the accuracy of the current fit, six parameters are required for the subdomain $0 < x \leq 1$, six additional parameters for the domain $1 < x \leq 4$, and 4 more parameters for the domain $x \geq 4$. Furthermore, each of those sixteen parameters is specified to seven or more digits of precision. The behavior when using the fit of Cody and Thatcher to compute higher-order E_n is also similar to that of the NBS; namely, errors become much larger, more quickly, because of the failure of Cody and Thatcher's

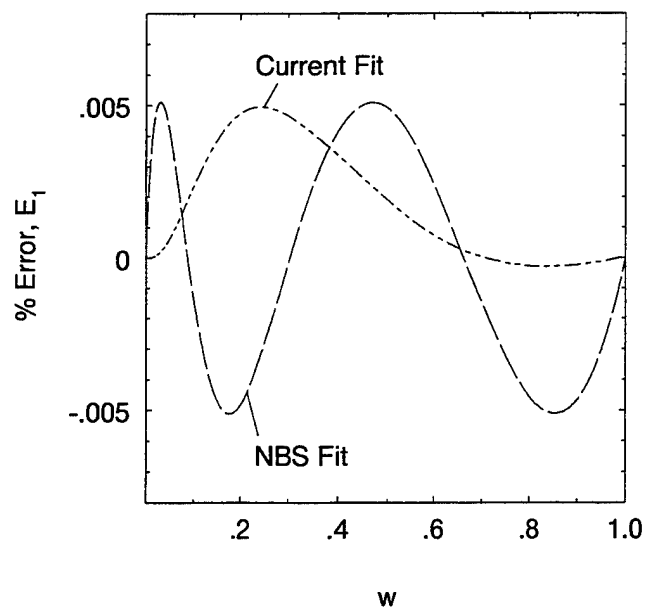


Figure 7. A comparison of the current fit to the four-parameter NBS fit, over the limited domain of $0 < w < 1$.

fit to asymptote to the proper limiting derivatives. This particular shortcoming of their fit can be circumvented, but only through the use of significantly greater number of parameters in the fit to the $x \geq 4$ subdomain.

5. Fitting Strategies

A few words may be in order here, on the formulation of fitting strategies for functions in general. With enough parameters, any function may be fit to a high degree of accuracy. The goal, however, is to achieve this fit, while minimizing the number of parameters and computational expense while, at the same time, maximizing the accuracy and the domain of applicability. Depending on how little or great an effort is warranted for the problem at hand, some or all of the following suggestions may be of utility in formulating an intelligent fit to a specified function, G , numerical values for which are known only in tabular form:

- 1) Compress the function's domain and range of interest to a manageable size (*i.e.*, analyze and fit a transformed function, H , if easier to digest than the original function, G).
- 2) Obtain limiting behaviors of the original (G) or transformed (H) function, if possible. This includes not only functional values, but slopes and higher derivatives. Such limits are needed if one wishes the fit to accurately converge in the limits of the domain.
- 3) Convert limiting behaviors into functional stencils (*e.g.*, $h_{small-x}$, $h_{large-x}$, $g_{asymptote}$, *etc.*). Often, the more derivatives that the stencil can match, the easier it will be to subsequently fit the transition function.
- 4) Develop a functional form for G or, if easier, for H (in terms of, hopefully, a single transition function, f) that is able to effectively transition between the limiting behaviors of the function. At this point, the unknowns are not individual fitted parameters, but instead the transition function(s). A simple example would be $H = f \cdot h_{small-x} + (1-f)h_{large-x}$. From this developed form,

quite a bit should be known about the general behavior of the transition function, f . For example, it might be known that $f(0)$ is 1, with an initial slope of -1, and which asymptotes at large x to 0.

5) Explicitly solve for tabulated values of the transition function, using the numerically integrated or tabulated values for G or H , and the calculated values for the stencils, $h_{small-x}$, etc. Using the above example, $f = (h_{large-x} - H)/(h_{large-x} - h_{small-x})$. The goodness of a particular functional form for G or H , in terms of f , may be assessed by observing how smoothly the calculated values of the f function behave. For example, it is generally easier to fit a monotonic transition function than one which oscillates. If the computed values for f don't seem to follow a desired (easily fitted) form, return to step 4 and reformulate a new functional form.

6) Based on observations of the behavior of the transition function, f , specify a specific form for the transition function in terms of parameters to be fit. For example, $f = A/x + Bx^2$. The observed behavior of the tabulated values for f should help in the specification of a good parameterized form.

7) Fit the parameters associated with the transition function. Ample numbers of coded programs exist to assist in this task, or else a simple (if inefficient) fitting routine may be written to minimize a specified error function (e.g., least squares).

8) Once the fitted parameters are obtained, evaluate the accuracy of the fit. If quality of fitted results are below expectations, return to step 6 or 4 to reformulate new trial functions.

In the current work of fitting E_1 , step 1 is accomplished by transforming both the domain (from x to w in eqn [7]) and the range (from E_1 to F_1 and eventually to $F_1 \cdot w$). In step 2, eqn (9) is employed to obtain the slope and derivatives of F for infinitesimal w and eqn (10) is used to express the analytically known behavior of E_1 for small x in terms of large w . Step 3 is accomplished by formulating the stencils $\ln[1+\ln(1+w)]$ for small w and $\ln(1+e^{-\gamma} w)$ for large w . Eqn (11) constitutes the functional form developed, as part of step 4. The transition function, f , is explicitly calculated, per step 5, and plotted in Figure 5 to reveal its desirable (easily fitted)

characteristics. The transition function is specified, in terms of parameters, in eqn (14), in accordance with step 6. Using a computational routine, the parameters to the transition function are fitted, as given in eqns (16), per step 7. The accuracy is evaluated and found acceptable, thus completing step 8 and the process.

This methodology may also be used to generate fits to experimental data, if something is analytically known about the physical process which created the data. In contrast to the methodology described here, polynomial fits are very popular (especially in the experimental community) because of the trivial cost in obtaining the fit. Unfortunately, polynomial fits are virtually guaranteed to offer zero extrapolative capacity beyond the domain over which they were fit. Furthermore, they offer zero insight into the physical behavior of the unknown function or data, and generally require many more parameters to achieve the same level of accuracy as an intelligent fit, as described here. And without some forethought, functions such as the exponential integrals are very costly to fit directly with polynomials because of their exponential nature [e.g., a truncated eqn (5) is essentially a very costly polynomial fit to the exponential integral].

In contrast to the polynomial fit, the process described here offers a logical methodology for generating fits to difficult functions or data, such that good results may be obtained with fewer parameters and at a reasonable cost. For an oft-used function, the extra effort required to compose an intelligent fit might very well be justified. A quote attributed to Cauchy, the 19th century mathematician, contends that "Give me five free parameters and I will give you the equations for an elephant, but give me a sixth free parameter and I will make the elephant wag its tail." Such versatility with so few parameters is surely possible only by way of an intelligent fit.

6. Summary

A compact (not piecewise), analytical fit has been developed for the class of integrals known as exponential integrals. The fit has been shown to match the numerically integrated

exponential integral, E_1 , to within an error of 0.0052%, over the complete domain of the function. Related integrals, E_2 and E_3 , were computed to within 0.029% and 0.15%, respectively, when using the current E_1 fit as part of the general E_n solution. Achieving such a feat is complicated by the fact that the value of these integrals, being exponential in nature, can change several-hundred orders of magnitude over a reasonably small section of the integral's domain.

By avoiding a series of piecewise fits to describe the complete domain of the function, it is guaranteed that the current fit is continuous in value, slope, and all higher derivatives. By contrast, a series of piecewise fits must either contend with discontinuous values, slopes, and/or higher derivatives, or else employ a smoothing algorithm to splice the piecewise fits. Such smoothing algorithms could be more computationally expensive than the fit itself and, therefore, need to be considered as part of the computational burden. Additionally, the avoidance of piecewise fitting permits the coding of the fit into a programming language without the use of conditional (*i.e.*, IF...THEN) statements. For some parallel-computing architectures, the use of conditional statements (required of piecewise fits) precludes maximum computing efficiency.

The ability to achieve a good fit, encompassing the complete domain of the function, with the use of only four parameters, stems completely from the fact that so much could be analytically deduced about the behavior of the function in large- x and small- x limits, prior to actually composing the form of the fit. In the small- x limit, the exact limiting form of the result is analytically known. In the large- x limit, a functional stencil that matches value, slope, and curvature of the actual exponential integral is employed. Furthermore, this stencil for the large- x (small- w) limit, given by $\ln[1+\ln(1+w)]$, does not numerically explode as w increases but, instead, smoothly fades as a diminishing percentage of the large- w (small- x) solution. In this manner, special accommodations (such as piecewise fitting of the solution) do not have to be made in order to transition from the small- w to large- w solution.

The accuracy of the fit exceeds a comparable (*i.e.*, four-parameter) fit published by the (former) U.S. National Bureau of Standards [5]. Furthermore, the NBS fit is accurate over only a specified subset of the functional domain. If the current fit is restricted to the same functional

subdomain as the NBS fit, only two parameters are required to significantly exceed the accuracy of the NBS fit. And because the NBS fit fails to properly match the limiting slope and higher-order derivatives of the exponential integral, E_1 , the use of the NBS fit to evaluate the higher-order E_n produces a greater limiting error than the current fit: over 120% in the case of E_3 , as compared with 0.15% by using the current fit. Similar results arise when comparing the current fit to the four-parameter fits of Cody and Thatcher [7], which are more recent than the NBS fits. However, if the number of parameters and piecewise nature of the fits are not issues, Cody and Thatcher still provide the most accurate of all fits. To achieve errors on the order of one part in 10^{20} , though, a total of 52 high-precision fitting parameters are required on their part.

The methodology used to generate the current fit was summarized in a loosely codified form. This methodology can be of assistance in generating fits to other difficult functions or even experimental data, if something is analytically known about the physical processes that created the data.

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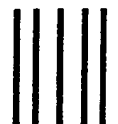
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